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ME469: Geometric Fidelity

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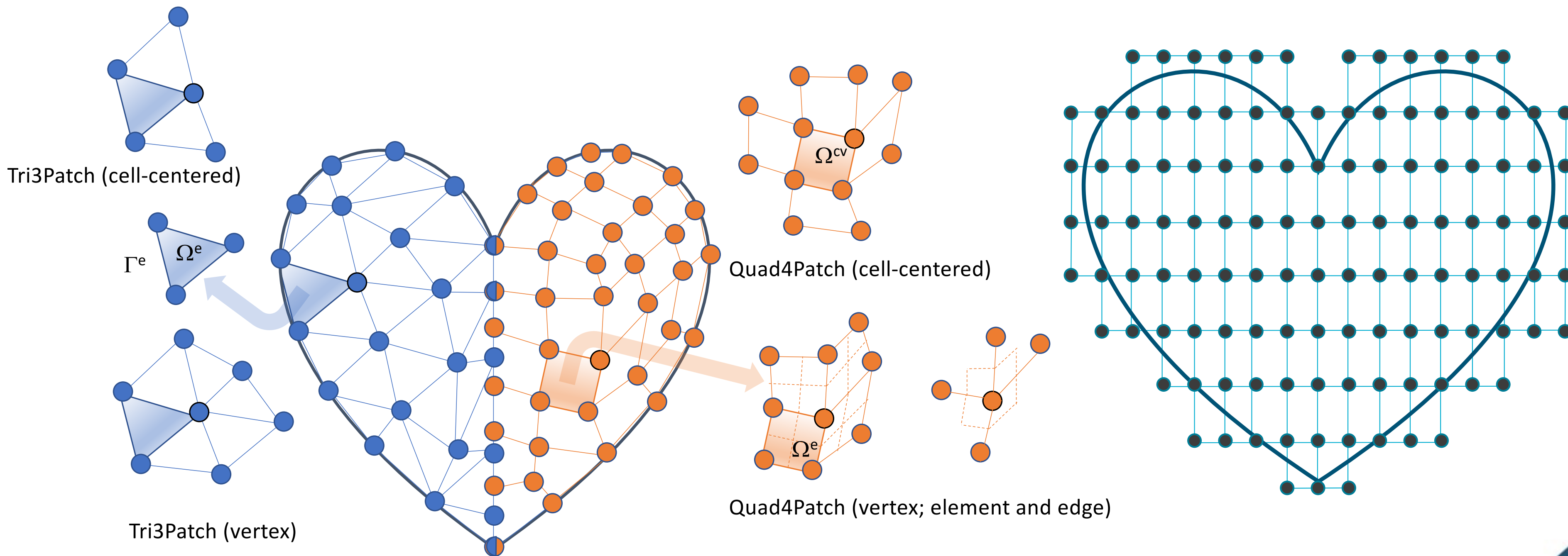
U.S. DEPARTMENT OF ENERGY

NNSA

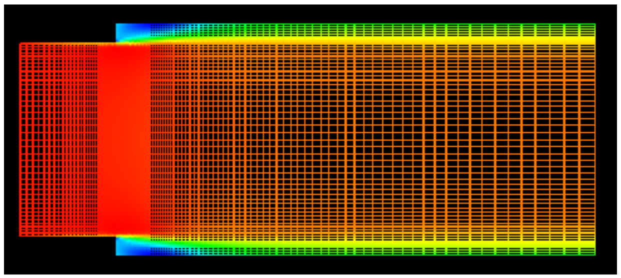
Review of Discretization Options

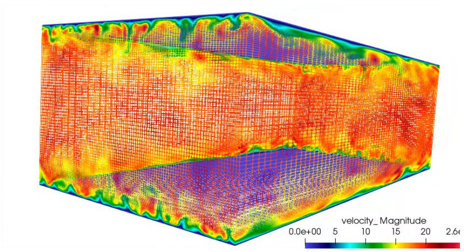
- Degree-of-freedom (DOF) for:
  - Cell-centered: Stencil is based on an element:face:element
  - DOFs at vertices of elements, or “nodes”, element:node (CVFEM, FEM), edge:node (EBVC)

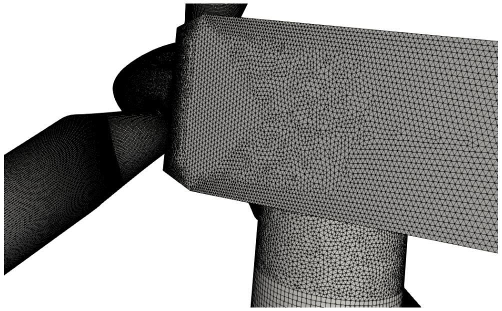


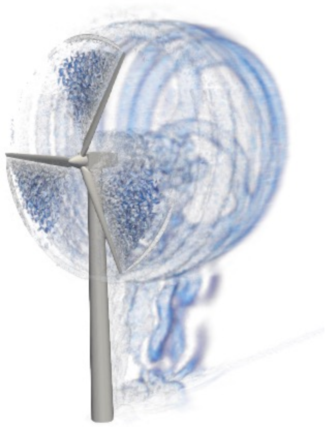
Simple vs Complex Domains

- Some Geometries are simple, while others are complex









Simple One-Dimensional Diffusion Example

Let us introduce (briefly) the Method of Manufactured Solutions (MMS)

- Consider a simple diffusion equation:

$$\frac{d^2\phi}{dx^2} = 0$$

with a presumed, or manufactured solution: $\phi^{MMS}(x) = x^2$

$$\frac{d^2\phi^{MMS}}{dx^2} = S^{MMS} = 2$$

Gauss-Divergence

$$\int \frac{d^2\phi^h}{dx^2} dV = \int S^{MMS} dV \qquad \int \frac{d\phi^h}{dx} dS = \int S^{MMS} dV$$

Discrete flux-based form at the sub-control volume surface (scs) and sub-control volume IP:

With error: $\epsilon = \phi^{MMS} - \phi^h$

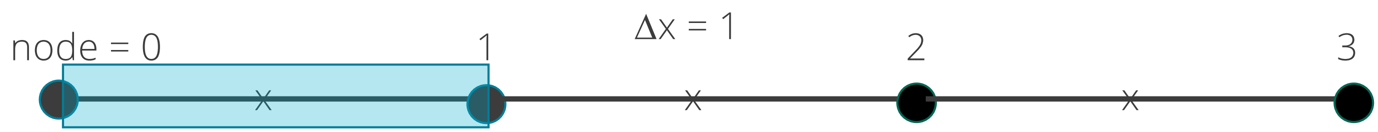
$$\sum_{scsIP} \frac{d\phi^h}{dx} A_{scsIP} = \sum_{scvIP} S^{MMS} V_{scvIP}$$

First....

- Let’s review matrix assembly from a previous lecture, with a focus on a verification “patch test”
- Recall, a linear basis was able to reconstruct a quadratic solution perfectly when the norm was computed at the degree of freedom locations

Simple One-D MMS Example; Edge-based Assemble of Diffusion

We will use a linear basis and solve this system over a small patch of linear bar elements



Recall, simplified equation with RHS from source term already provided

$$\sum_{scsIP} \frac{d\phi^h}{dx}_{scsIP} = \sum_{scvIP} S^{MMS} \frac{\Delta x}{2}$$

Iterate elements with a simple left-hand side rule: += L and -=R

(note implicit conservation statement)

$$\frac{d\phi^h}{dx}_{scsIP} = \frac{\phi_1^h - \phi_0^h}{\Delta x} + C_0(\Delta x) + ...$$

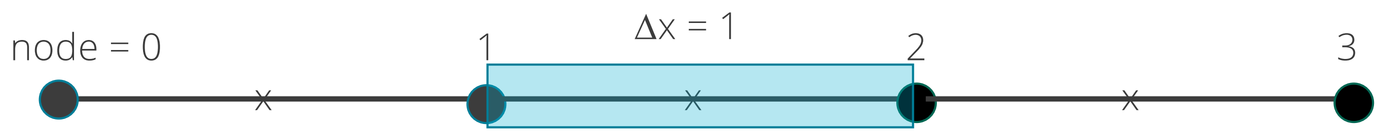
$$LHS_0 + = \frac{\phi_1^h - \phi_0^h}{\Delta x}$$

$$LHS_1 - = \frac{\phi_1^h - \phi_0^h}{\Delta x}$$

Edge 1

Simple One-D MMS Example; Edge-based Assemble of Diffusion

We will use a linear basis and solve this system over a small patch of linear bar elements



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Iterate elements with a simple left-hand side rule: += L and -=R

(note implicit conservation statement)

$$\frac{d\phi^h}{dx}_{scsIP} = \frac{\phi_2^h - \phi_1^h}{\Delta x} + C_0(\Delta x) + \ldots$$

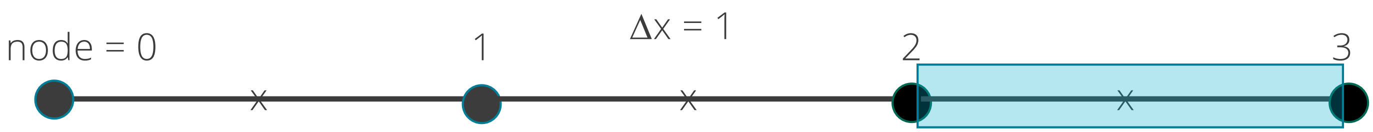
$$LHS_1 + = \frac{\phi_2^h - \phi_1^h}{\Delta x}$$

$$LHS_2 - = \frac{\phi_2^h - \phi_1^h}{\Delta x}$$

Edge 2

Simple One-D MMS Example; Edge-based Assemble of Diffusion

We will use a linear basis and solve this system over a small patch of linear bar elements



Recall, simplified equation with RHS from source term already provided

$$\sum_{scsIP} \frac{d\phi^h}{dx}_{scsIP} = \sum_{scvIP} S^{MMS} \frac{\Delta x}{2}$$

Iterate elements with a simple left-hand side rule: += L and -=R

(note implicit conservation statement)

$$\frac{d\phi^h}{dx}_{scsIP} = \frac{\phi_3^h - \phi_2^h}{\Delta x} + C_0(\Delta x) + \ldots$$

$$LHS_2 + = \frac{\phi_3^h - \phi_2^h}{\Delta x}$$

$$LHS_3 - = \frac{\phi_3^h - \phi_2^h}{\Delta x}$$

Edge 3

Simple One-D MMS Example; Collect all of the terms

$$LHS_0+ = \frac{\phi_1^h - \phi_0^h}{\Delta x}$$

$$LHS_1- = \frac{\phi_1^h - \phi_0^h}{\Delta x}$$

$$LHS_1+ = \frac{\phi_2^h - \phi_1^h}{\Delta x}$$

$$LHS_2- = \frac{\phi_2^h - \phi_1^h}{\Delta x}$$

$$LHS_2+ = \frac{\phi_3^h - \phi_2^h}{\Delta x}$$

$$LHS_3- = \frac{\phi_3^h - \phi_2^h}{\Delta x}$$

$$A = \frac{1}{\Delta x}\begin{bmatrix} -1 & +1 & 0 & 0 \\ +1 & -2 & +1 & 0 \\ 0 & +1 & -2 & 1 \\ 0 & 0 & +1 & -1 \end{bmatrix}$$

Fully assembled matrix

$$\frac{1}{\Delta x}\begin{bmatrix} -1 & +1 & 0 & 0 \\ +1 & -2 & +1 & 0 \\ 0 & +1 & -2 & 1 \\ 0 & 0 & +1 & -1 \end{bmatrix}\begin{bmatrix} \phi_0 \\ \phi_1 \\ \phi_2 \\ \phi_3 \end{bmatrix} = \begin{bmatrix} 2 \\ 2 \\ 2 \\ 2 \end{bmatrix}$$

Fully assembled system

$$\frac{1}{\Delta x}\begin{bmatrix} +1 & 0 & 0 & 0 \\ +1 & -2 & +1 & 0 \\ 0 & +1 & -2 & 1 \\ 0 & 0 & 0 & +1 \end{bmatrix}\begin{bmatrix} \phi_0 \\ \phi_1 \\ \phi_2 \\ \phi_3 \end{bmatrix} = \begin{bmatrix} 0 \\ 2 \\ 2 \\ 9 \end{bmatrix}$$

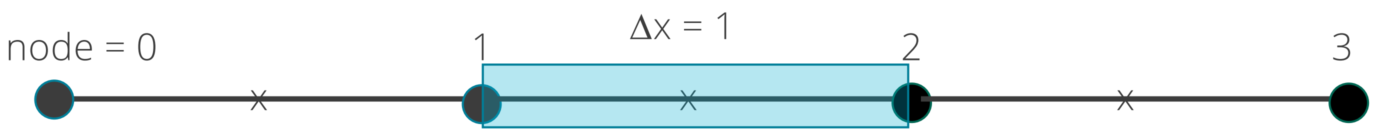
Correct for BCs

$$\phi^h = \begin{bmatrix} 0 \\ 1 \\ 4 \\ 9 \end{bmatrix}$$

Solution is exact….. Linear basis exactly captures a quadratic solution

Simple One-D Advection; Edge-based Assembly

Similar approach: Iteration of edges, definition of Left and Right node, etc.



$$\int w \frac{\partial \rho u_j \phi}{\partial x_j} dV \approx \sum_{ip} (\rho u_j)_{ip} \phi_{ip} n_j dS \approx \sum_{ip} \dot{m}_{ip} \phi_{ip}$$

$$\dot{m}_{ip} = \rho u_j n_j dS|_{ip} = \rho u_j A_j|_{ip}$$

We may also create a local matrix data structure, A[4]: With:

- A[0] += lhsFac (row node 1, "central-coeff")
- A[1] += lhsFac (row node 1, "east-coeff")
- A[2] -= lhsFac (row node 2, "west-coeff")
- A[3] -= lhsFac (row node 2, "central-coeff")

$$LHS_1 + = \frac{\dot{m}}{2}\left(\phi_2^h + \phi_2^h\right)$$

$$LHS_2 - = \frac{\dot{m}}{2}\left(\phi_1^h + \phi_2^h\right)$$

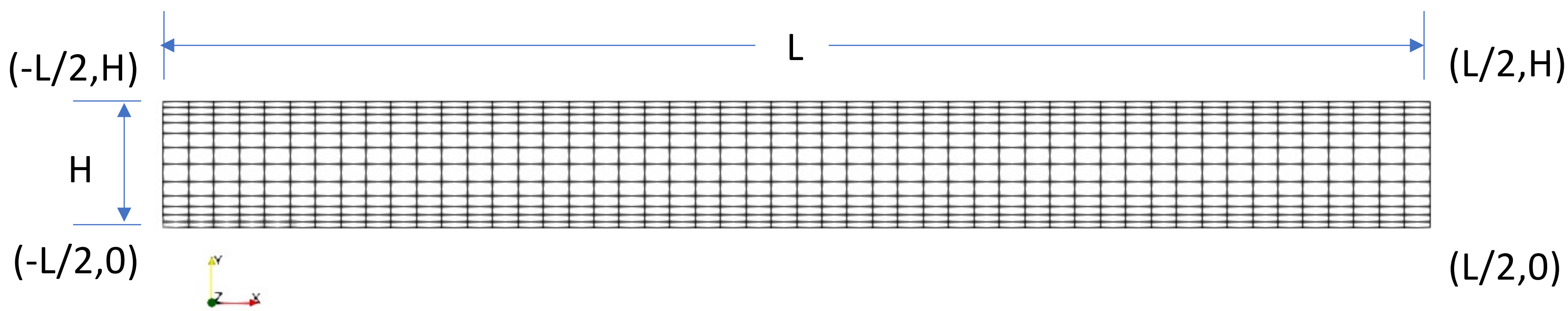
With: $lhsFac = \frac{\dot{m}}{2}$

Edge 2

Let's Revisit a Classic 2-dimensional Channel Flow (laminar)

This is the 2d_quad4_channel laboratory:
https://github.com/NaluCFD/Nalu/blob/master/reg_tests/test_files/laboratory/2d_quad4_channel/write_up/2d_quad4_channel_laboratory.pdf

- No-slip (walls) top and bottom
- Periodic (left and right) with a constant body force ...or... Open (left and right pressure drop)



Derivation

3.1 Analytical Velocity Profile

Given the assumptions provided in the introduction, the streamwise velocity equation reduces to,

$$\frac{dP}{dx} = \mu \frac{d^2 u_x}{dy^2}. \tag{4}$$

This equation can be integrated twice to obtain,

$$u_x(y) = \frac{1}{\mu}\frac{dP}{dx}\frac{y^2}{2} + k_1 y + k_2, \tag{5}$$

where k_1 and k_2 are constants of integration that are obtained through the application of boundary conditions, $u_x(y=0)=0$ and $u_x(y=H)=0$. Therefore, the final expression for the streamwise velocity is,

$$u_x(y) = \frac{1}{2\mu}\frac{dP}{dx}\left[y^2 - Hy\right]. \tag{6}$$

The above equation can be used to determine the vertical location at which the maximum velocity is found via solving $\frac{du_x}{dy} = 0$, or u_x^{max} occurs at $H/2$. The functional form for the maximum velocity is,

$$u_x^{max} = \frac{1}{8\mu}\frac{dP}{dx}H^2. \tag{7}$$

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Sizing

- Let's run at Re_τ=10

Reynolds number:

- Ratio of inertial to viscous forces

$$Re_D = \frac{\rho u D}{\mu}$$

- In this channel, define Reynolds number based on the wall friction velocity, u_τ (at H/2 length scale)

$$Re_\tau = \frac{\rho u_\tau H/2}{\mu}$$

4 Results

Let us test a simulation in which the Reynolds number based on wall friction velocity, u^τ, and half-channel height $H/2$, is ten: $Re^\tau = 10$. By constraining the Reynolds number, wall friction velocity, and density, the consistent viscosity is obtained via,

$$\mu = \frac{\rho u^\tau H}{2Re^\tau}. \tag{8}$$

To obtain the required pressure gradient, we exercise the relationship,

$$u^\tau = \sqrt{\frac{\tau_w}{\rho}}, \tag{9}$$

along with global momentum balance,

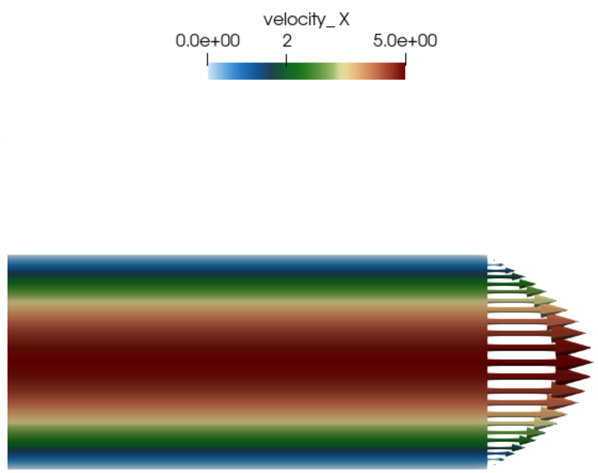
$$\int \frac{dP}{dx} dV = \int \tau_w dA, \tag{10}$$

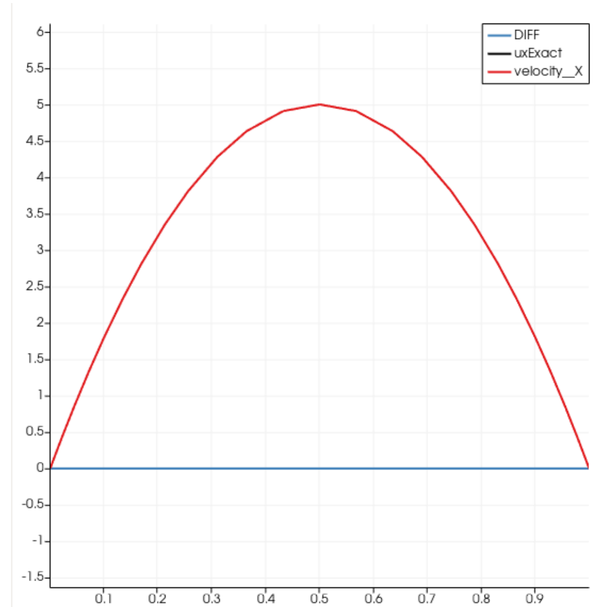
with $dV = LH$ and $dA = 2L$, to obtain the relationship between required pressure gradient and wall shear stress, $\frac{dP}{dx} = 2\tau_w$.

Simulation Results

Analytical Expression:

$$u_x(y) = \frac{1}{2\mu}\frac{dP}{dx}\left[y^2 - Hy\right].$$



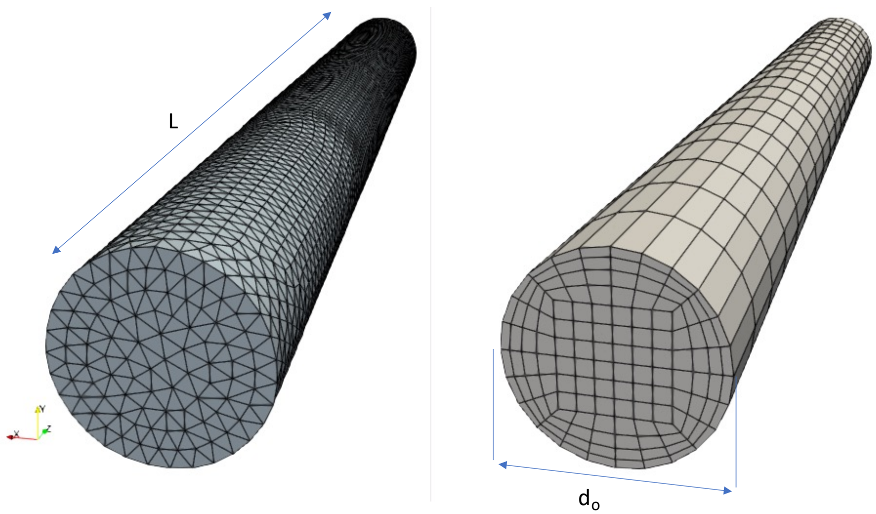


Zero Error when evaluating the norm at the nodes (in general, we may integrate over a domain and choose integration points that are not *nodally-lumped*

Let’s Revisit a Classic 3-dimensional Pipe Flow (laminar)

This is the 3d_tet4_pipe laboratory:
https://github.com/NaluCFD/Nalu/tree/master/reg_tests/test_files/laboratory/3d_tet4_pipe/write_up

- No-slip (walls) outer pipe
- Periodic (left and right) with a constant body force ...or... Open (left and right pressure drop)
- We have Tet4 (left) and a Hex8 (right) mesh



Derivation

3.1 Analytical Velocity Profile

Given the assumptions provided in the introduction, the axial momentum equation reduces to,

$$\frac{dP}{dz} = \frac{1}{r}\frac{\partial r \tau_{\tau_{rz}}}{\partial r}, \tag{11}$$

where $\tau_{rz} = \mu \frac{\partial u_z}{\partial r}$. Integration once results in the following equation,

$$\frac{r^2}{2}\frac{dP}{dz} = r\mu\frac{\partial u_z}{\partial r} + k_1, \tag{12}$$

which, based on $\frac{\partial u_z}{\partial r} = 0$ at the centerline $r = 0$, yields $k_1 = 0$. A second integration results in,

$$u_z(r) = \frac{r^2}{4\mu}\frac{dP}{dz} + k_2. \tag{13}$$

Applying $u_z(r = R) = 0$, yields the following expression for the axial velocity as a function of radial position,

$$u_z(r) = \frac{1}{4\mu}\frac{dP}{dz}\left[r^2 - R^2\right]. \tag{14}$$

The above equation can be used to determine the location at which the maximum velocity is found via solving $\frac{du_z}{dr} = 0$, or u_z^{max} occurs at $r = 0$. The functional form for the maximum velocity is,

$$u_x^{max} = -\frac{R^2}{4\mu}\frac{dP}{dZ}. \tag{15}$$

Sizing

- Let's run at Re_τ=20

Reynolds number:

- Ratio of inertial to viscous forces

$$Re_D = \frac{\rho u D}{\mu}$$

- In this channel, define Reynolds number based on the wall friction velocity, u_τ (at d_o length scale)

$$Re_\tau = \frac{\rho u_\tau d_o}{\mu}$$

4 Results

Let us test a simulation in which the Reynolds number based on wall friction velocity, u^τ, and diameter of the pipe (0.02 m) is $Re^\tau = 20$. In this mesh configuration, the length L is 0.2 m. By constraining the Reynolds number, wall friction velocity, and density, the consistent viscosity is obtained via,

$$\mu = \frac{\rho u^\tau d_o}{Re^\tau}. \tag{16}$$

To obtain the required pressure gradient, we exercise the relationship,

$$u^\tau = \sqrt{\frac{\tau_w}{\rho}}, \tag{17}$$

along with global momentum balance,

$$\int \frac{dP}{dz} dV = \int \tau_w dA, \tag{18}$$

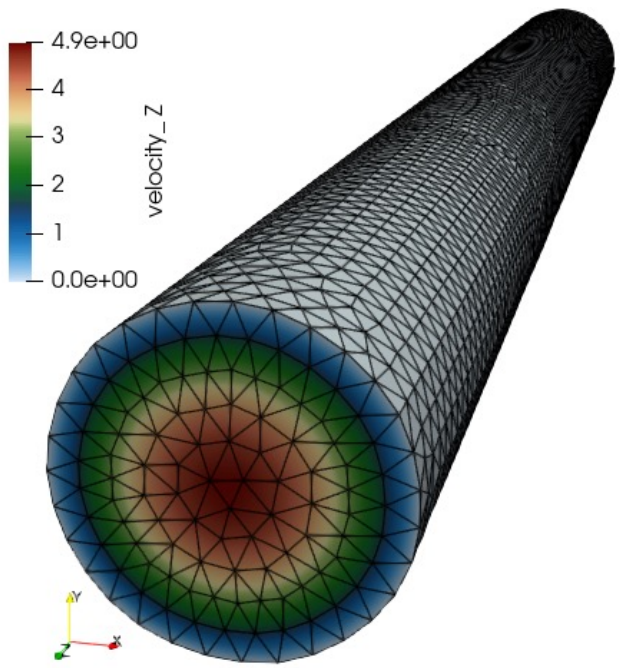
with $dV = \pi r^2 L$ and $dA = 2\pi r L$, to obtain the relationship between required pressure gradient and wall shear stress, $\frac{dP}{dz} = 2\frac{\tau_w}{r}$.

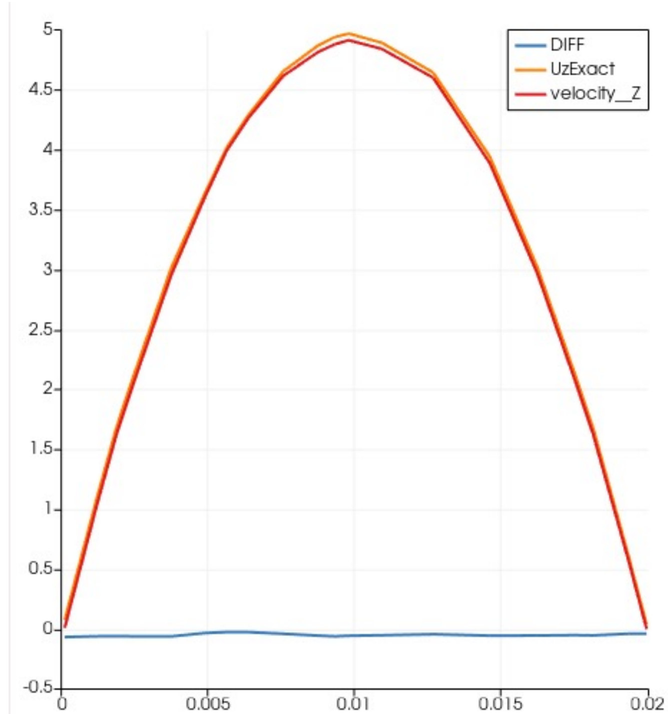
Simulation Results

Analytical Expression:

$$u_z(r) = \frac{1}{4\mu}\frac{dP}{dz}\left[r^2 - R^2\right].$$

Non-zero error when evaluating the norm at the nodes…





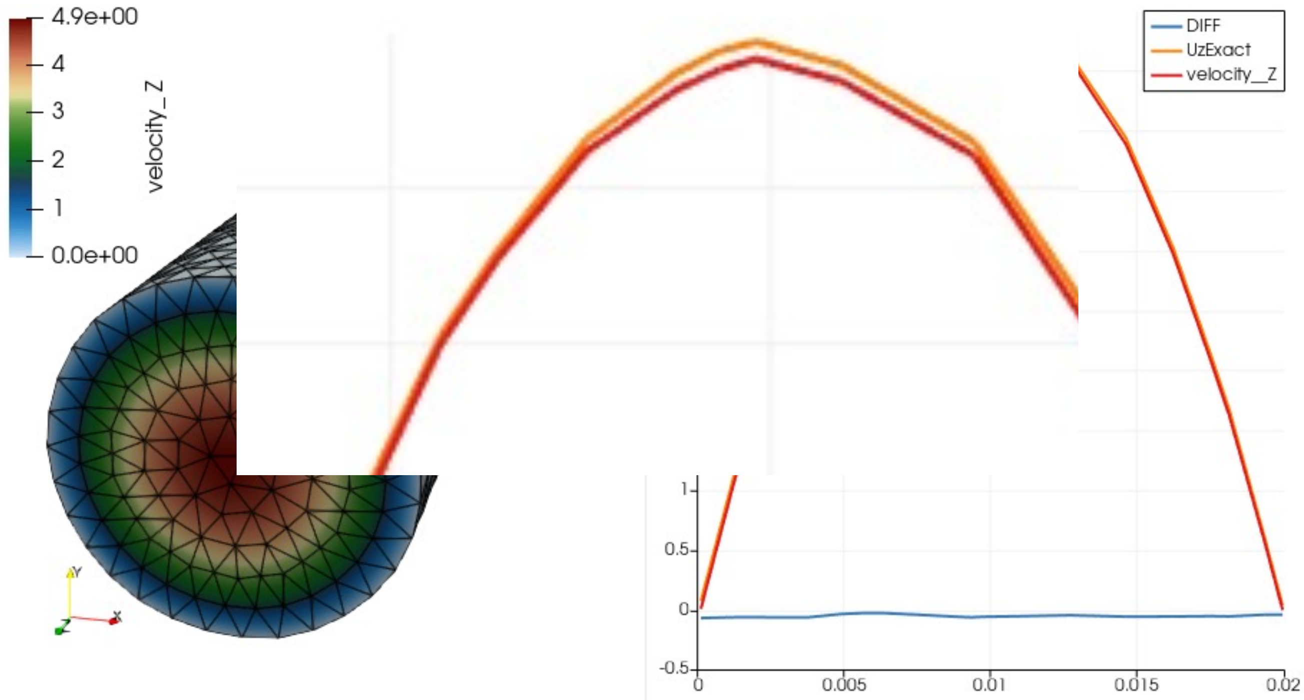
Simulation Results

Analytical Expression:

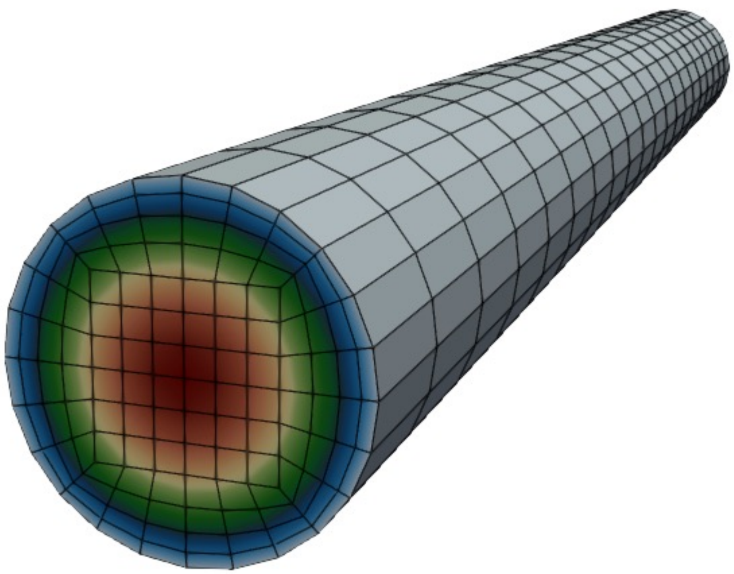
$$u_z(r) = \frac{1}{4\mu}\frac{dP}{dz}\left[r^2 - R^2\right].$$

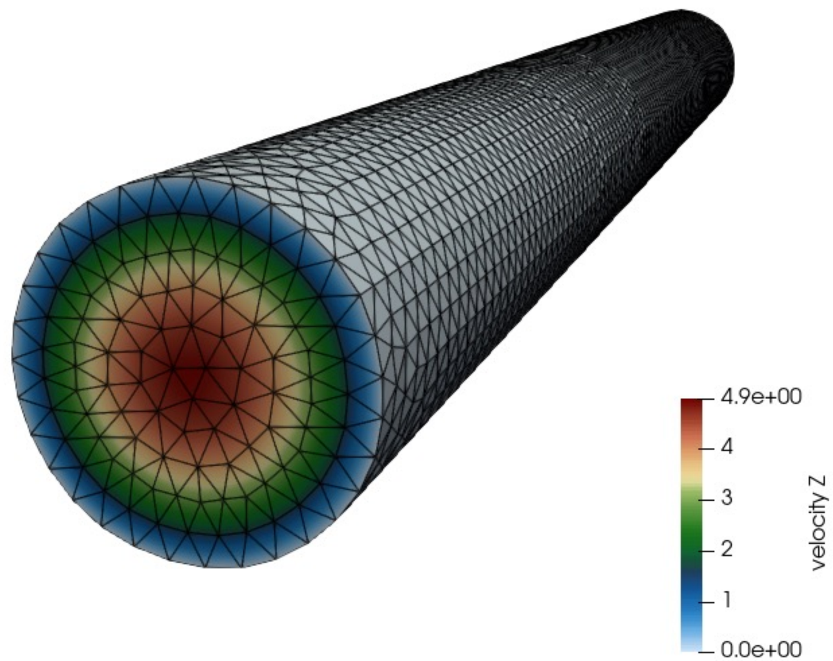
Non-zero error when evaluating the norm at the nodes…

What happened?



What About Tet4 vs Hex8?





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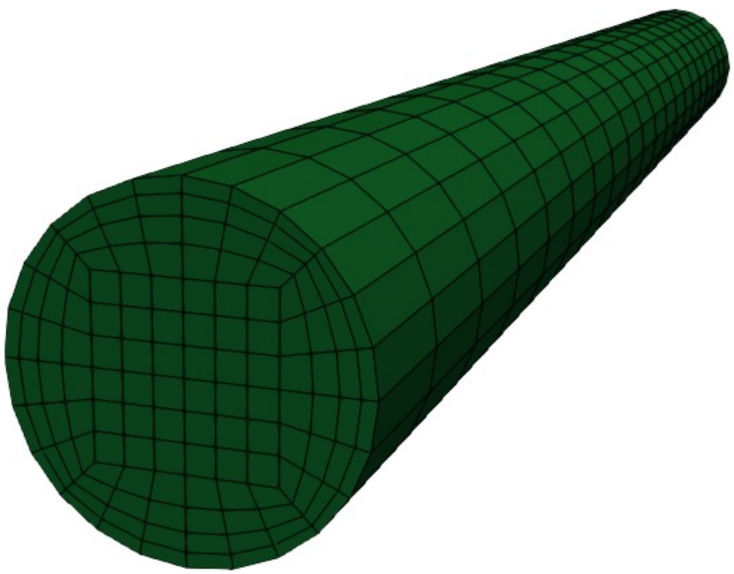
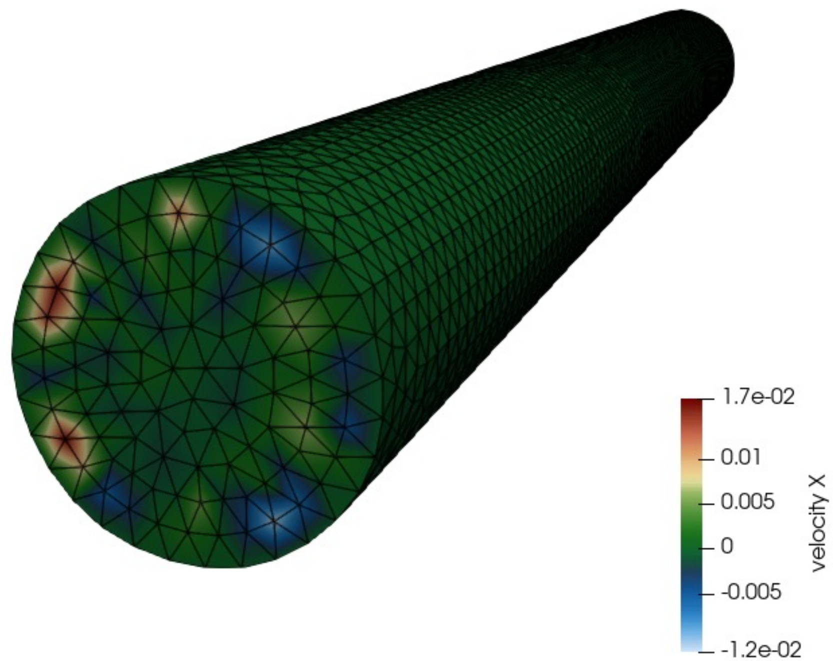
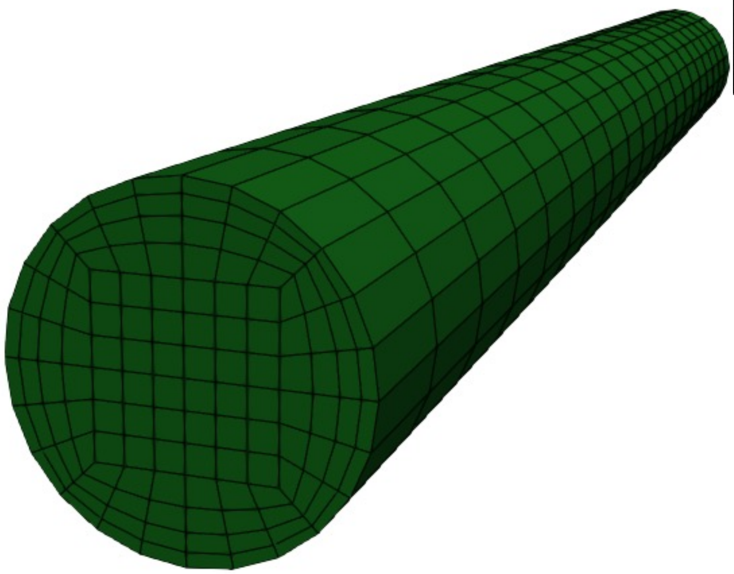


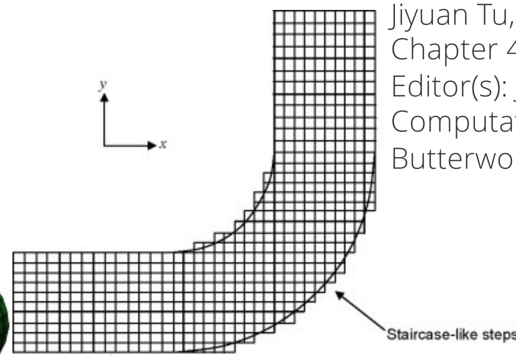


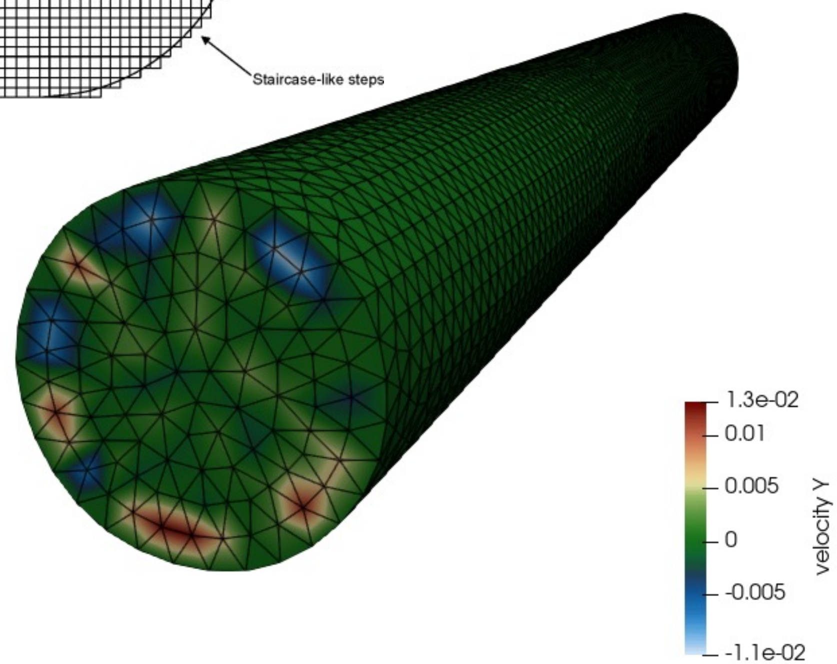
~0.3% error in non-streamwise velocity components in the tet-based result, ~0% for Hex8!!!

What About Tet4 vs Hex8?

Jiyuan Tu, Guan-Heng Yeoh, Chaoqun Liu,
Chapter 4 - CFD Mesh Generation: A Practical Guideline,
Editor(s): Jiyuan Tu, Guan-Heng Yeoh, Chaoqun Liu,
Computational Fluid Dynamics (Third Edition),
Butterworth-Heinemann, 2018, Pages 125-154,







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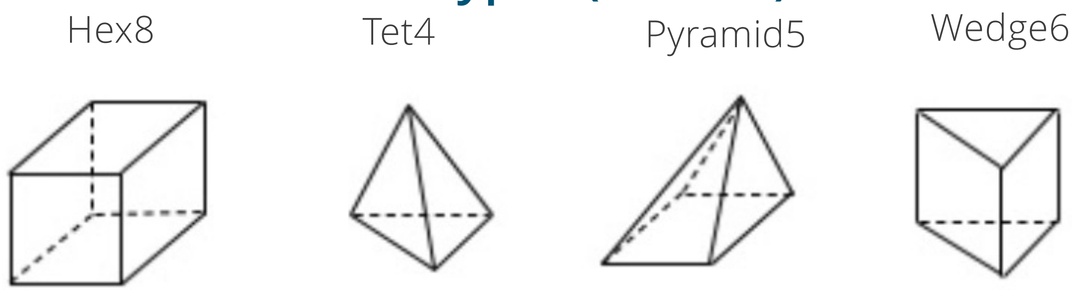
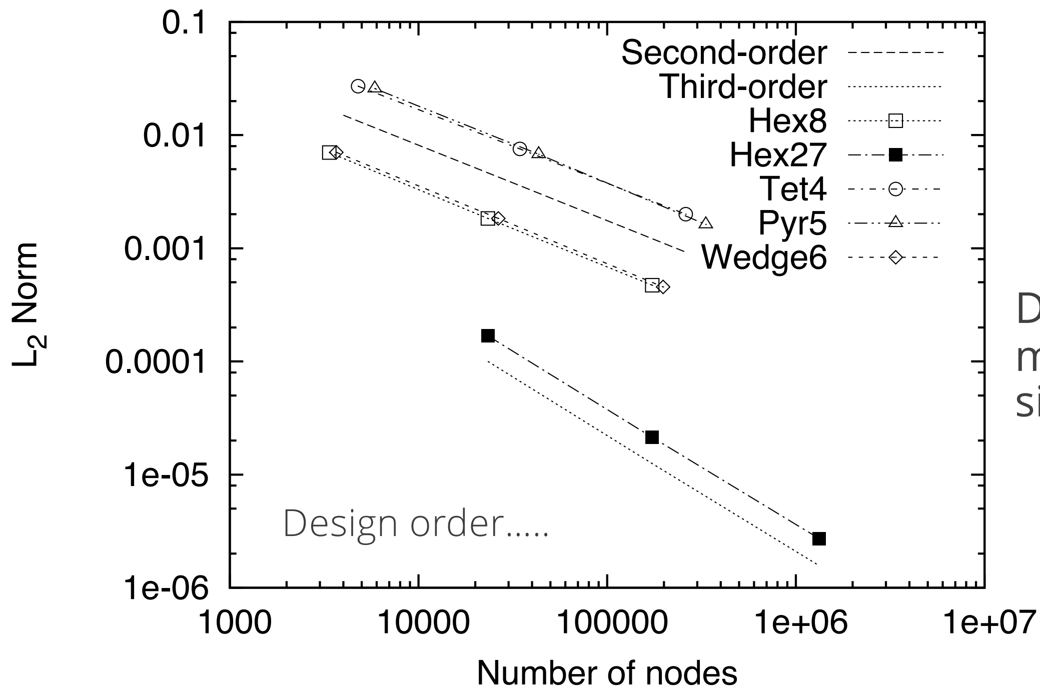
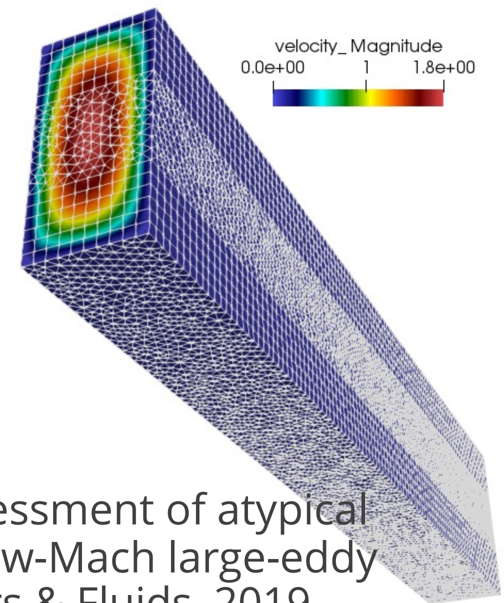
Unstructured Mesh Types (Review) and Results







Domino et al., “An assessment of atypical mesh topologies for low-Mach large-eddy simulation”, Computers & Fluids, 2019

$$u_z = -\frac{1}{2\mu}\frac{dp}{dz}\left[b^2 - y^2 - \frac{4}{b}\sum_{n=0}^{\infty}(-1)^n \frac{1}{m^3}\frac{\cos(my)\cosh(mx)}{\cosh(ma)}\right]$$

Conclusions

- Geometric fidelity for curved surfaces can be very important
- Unstructured meshing generally affords easier meshing, with increase throughput (especially when simulating complex geometries)
- Hex-based errors may be lower than Tet-based simulation results, however, balanced with ease of meshing
- The key is that all methods are “design-order”, i.e., demonstrate expected reduction of errors as a function of mesh size